Ethanone, 1-(2,4-dihydroxyphenyl)-89-84-9 | DTXSID4058998

89-84-9 DTXSID4058998

Model Performance

Model	Data	
IVIOGEI	Dala	

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 3.01

Global applicability domain: Inside

Local applicability domain index: 4.75e-01

Confidence level: 7.55e-01

Nearest Neighbors from the Training Set

Image not found

Sulfolane

Measured: 7.08 Predicted: 6.91

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2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00 Predicted: 1.47

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1,1'-Oxybis-2-propanol

Measured: 4.57 **Predicted:** 3.83

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Triethyl phosphate Measured: 1.29 Predicted: 1.38

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2,2-Dimethylpropane-1,3-diol

Measured: 4.68 Predicted: 4.44